FINAL REPORT

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Direct Methods for the Solution of Systems of Linear Equations with Sparse Coefficient Matrix and Related Topics

by

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1. Introduction.

In this report, a concise summary of the research work done in connection with the NASA Grant NGR-33-015-013 for the period December 1, 1967 to August 31, 1970 is given. The period from June 1, 1965 to November 31, 1967 has already been covered in [4]. The research has lead to 41 publications and reports, 4 contributed papers and one lecture. Furthermore, the principal investigator has been invited to present some of his research results at six professional meetings in U.S. and abroad. Since [1]-[3], [5]-[10] and [14] have been covered in [4], we give a summary of the work described in the remaining publications.

2. Summaries of Publications and Reports.

In [11] a geometrical as well as some graph theoretic interpretations are given to the currently known techniques for minimizing the densities of the product form of inverses of sparse matrices in linear programming. It is shown how such interpretations lead to improved techniques in the probabilistic updating of the row count vector and the a priori determination of the density measures associated with the columns of the given matrix. It is also shown how some of the above techniques can be applied to the orthogonalization methods for the inversion of sparse matrices. For example, in the Gram-Schmidt process if a density measure is associated with each column of the given matrix then the density of the resulting orthogonal matrix can be minimized by orthogonalizing the columns in the ascending order of the density measures. Some results of the computational experiments using the above techniques for both the elimination and the orthogonalization methods are given.

A new formulation of the ascent algorithm for the Chebyshev solution of linear systems is given in [12]. This leads to two algorithms, which are similar to the ordinary simplex and the product form of inverse algorithms for the solution of linear programming problems.

In [13], a method for computing the generalized inverse of a matrix is described, which makes use of elementary orthogonal matrices and the Gaussian elimination. The method also yields orthonormal bases for the ranges and the null spaces of the matrix and the generalized inverse. Modifications of the method for the solution of simultaneous linear equations are given. Compact storage schemes, in the case of sparse matrices, are also described.

A characterization of various generalized inverses and a constructive proof of the weak method of steepest descent for the least squares solution of a system of linear equations is given in [15].

In [16] homogeneous, ill-conditioned and singular linear equations are considered and some techniques for improving their conditioning and methods for solution are described.

An algorithm is given in [17] for minimizing the number of non-zero elements created during the forward course of the Crout reduction (no new elements are created in the back substitution). Practical computational techniques for the efficient utilization of the algorithm are also discussed.

In [18], an algorithm for computing Chebyshev solution of $n + 1$ inconsistent linear equations in n unknowns is given. It makes use of orthogonal triangularization followed by the backsubstitution part of the Gaussian elimination. The general case, of m equations in n unknowns where $m > n$ is considered in [19]. An algorithm is given there, which is similar to the Revised Simplex method of linear programming, and is a consequence of a reformulation of the Ascent algorithm and the use of Generalized inverses.

An iterative method for the solution of a system of simultaneous linear equations, having a singular coefficient matrix is described in [20].

The method is obtained by minimizing (in the least squares sense) the image under the transpose of the coefficient matrix of a given residual vector.

In [21], we have discussed the problem of minimizing the number of new non-zero elements created during the forward course (no new elements are created in the back substitution) of the Gaussian elimination for the solution of sparse equations. A pivot choice that leads to the minimum number of new non-zero elements under a convexity assumption is given. Some other methods for the determination of near optimum pivot choices are also described.

A unified derivation of various minimization algorithms which use the notion of updating an estimate of the inverse of the Hessian matrix is given in [22]. A new method for updating the estimated inverse of the Hessian matrix and a simple technique for making computational improvements in the various algorithms are also given.

The problem of minimizing the number of zero elements that become non-zero during the computation when a sparse symmetric matrix is reduced to a triple diagonal form, either by Givens' or Householder's method, is discussed in [23]. Algorithms for minimizing the growth of such non-zero elements are given.

In [24], a characterization of $A^{+}_{V,W}$ (the V-W generalized inverse of a matrix A) is given. This not only leads to a simple method for computing $A^{+}_{V,W}$ but also yields the basis and the projections for the ranges, as well as the null spaces of A and $A^{+}_{V,W}$. A method which improves the computation of $A^{+}_{V,W}$ is described. Applications of the V-W generalized inverse in the solution of linear equations and the construction of test matrices are also given.

A survey of the currently known direct methods for evaluating the inverse of sparse matrices, solution of systems of linear equations having sparse coefficient matrices, and the determination of eigenvalues of such matrices is given in [25].

In [26], the " a priori " permutation of the rows and columns of the coefficient matrices of large sparse linear systems, such that the resulting matrices are in forms which are desirable from the view point of the Gaussian elimination, is discussed. Symmetric permutations, which lead to band form (BF), doubly bordered band form (DBBF), or doubly bordered block diagonal form (DBBDF), are considered in detail. Several properties of matrices in BF, DBBF and DBBDF are derived by making use of a probabilistic approach. It is then shown how this information can be efficiently utilized for transforming an arbitrary sparse matrix to BF, DBBF or DBBDF. An algorithm for this purpose is described and a graph theoretic interpretation for it is given. This algorithm should be especially useful when many problems with similar pattern of non-zero elements but with differing values have to be solved. The paper concludes with a brief survey of the currently known methods for minimizing the band width of large sparse matrices.

The problem of minimizing the number of zero elements that become non-zero during the computation, when a large sparse matrix is reduced to the Hessenberg (almost triangular) form by Gaussian similarity transformations, is discussed in [27]. Algorithms for minimizing the growth of such non-zero elements are given.

For a system of simultaneous linear equations $Ax=b$, where A is a rectangular matrix of rank σ, an improvement in the conditioning of A is suggested. If $B=A + \epsilon (A^T)^+$, and $C = B + \epsilon (A^T)^+ B^+ (A^T)^+$, then it is shown that $\mathrm{cond}(C) \leq \mathrm{cond}(B) \leq \mathrm{cond}(A)$ provided $0 < \epsilon^2 + \epsilon < \mu^4_{\sigma}$, where μ_{σ} is the least non-zero singular value of A. Furthermore, it is shown that the minimum least squares solution of $Cx=b$ is the same as least squares solution of the equivalent system $\hat{A}x=\hat{b}$, where $\hat{A} = (A | \sqrt{\epsilon}\, \nabla)^T$, $\nabla^2 = I + \Delta^{-1}$ and $\Delta = A^T A + \epsilon I$, which avoids the computation of A^+ and B^+.

In [29], a method for partitioning non-singular sparse matrices into block forms is given. The method utilizes the concepts of pseudo-Boolean programming and graph theory.

Two new methods for computing the generalized inverses are given in [30]. The formulas given in this paper are somewhat simpler and in certain cases involve less work than similar methods available in the literature.

3. Conclusions.

In view of the above mentioned publications it is evident that significant savings in time and computing effort are possible in computations involving sparse matrices if suitable row-column permutations are performed on them. This extends the size and scope of the problems that can be solved on the present generation of computers. It is now fairly easy to find the generalized inverse of a matrix and the least squares solution of equations, as several algorithms are available for this purpose, some of these were developed as a result of this grant. Similarly, the determination of the Chebyshev solution of a system of equations is now a reasonably easy problem in view of the algorithms developed here and elsewhere.

PUBLICATIONS

1. On the Product Form of Inverses of Sparse Matrices, SIAM Rev., 8 (1966), pp. 336-342. Reviewed in Math. Rev., 34 (1967), 8631; Comp. Rev., 9 (1968), 14,306.

2. On the Product Form of Inverses of Sparse Matrices and Graph Theory, SIAM Rev., 9, (1967), pp. 91-99. Reviewed in Math. Rev., 36, (1968), 1092; Zbl. Math., 168(1969), 133.

3. Product Form of Inverses of Sparse Matrices, NASA-CR-69270, (1965), 11 pp.

4. Product Form of Inverses of Sparse Matrices and Related Topics, NASA-CR--90534 (1967), 7 pp.

5. On Row-Column Permutation of Sparse Matrices, Computer J. 10, (1967), pp. 300-305. Reviewed in Comp. Rev., 9 (1968), 14, 307; Math. Rev., 36 (1968), 1091; Zbl. Math., 155(1968), 469.

6. A Direct Method for Generalized Matrix Inversion, SIAM J. on Num. Anal., 4, (1967), pp. 499-507. Reviewed in Comp. Rev., 9 (1968), 14,995; Math. Rev., 36 (1968), 2309; Zbl. Math., 153(1968), 461.

7. Solution of a System of Simultaneous Linear Equations with a Sparse Coefficient Matrix by Elimination Methods, Nord. Tids. Inf. Bhld., (BIT) 7, (1967), pp. 226-239. Reviewed in Comp. Rev., 9 (1968), 13,863; Math. Rev., 36 (1968), 2308.

8. A Computational Method for Evaluating Generalized Inverses, Computer J., 10, (1968), pp. 411-413. Reviewed in Comp. Rev., 9 (1968), 15,435; Math. Rev., 36 (1968), 4793; Zbl. Math., 167 (1969), 156.

9. Solution of Linear Equations with Coefficient Matrix in Band Form, Nord. Tids. Inf. Bhld. (BIT), 8 (1968), pp. 53-58. Reviewed in Comp. Rev., 9 (1968), 15,431; Math. Rev., 37 (1969), 2425; Zbl. Math., 157(1969), 225.

10. On the Orthonormalization of Sparse Vectors, Computing, 3 (1968), pp. 268-279. Reviewed in Comp. Rev., 10 (1969), 17521. Zbl. Math. , 174, 2(1969), 468; Math. Rev., 39(1970), 1103.

11. The Elimination and the Orthogonalization Methods for the Inversion of Sparse Matrices, Advancing Frontiers in Operational Research (proceedings of International seminar, 7-10 August 1957, New Delhi) Eds. H. S. Subba Rao, N. K. Jaiswal & A. Ghosal, Hindustan Publishing Co. New Delhi 1969, pp. 315-334.

12. On Chebyshev Solution of Inconsistent Linear Equations, Nord. Tids. Inf. Bhld. (BIT), 8 (1968), pp. 232-242.

13. On Computing Generalized Inverses, Computing, 4 (1969), pp. 139-152. Reviewed in Zbl. Math., 182(1970), 212.

14. On Projection Methods for Solving Linear Systems, Computer J., 12 (1969), pp. 78-81. Reviewed in Zbl. Math., 164(1969), 461; Math. Rev., 39(1970), 1104.

15. On Some Representations of Generalized Inverses, SIAM Rev., 11 (1969), pp. 272-276. Reviewed in Zbl. Math., 175(1969), 458.

16. Some Comments on the Solution of Linear Equations, (with B. Ramnath), Nord. Tids. Inf. Bhld. (BIT), 9 (1969), pp. 167-173. Reviewed in Comp. Rev., 10(1969), 18079.

17. The Crout Reduction for Sparse Matrices, Computer J., 12 (1969) pp. 158-159. Reviewed in Zbl. Math., 182(1970), 213.

18. Minimax Solution of n + 1 Inconsistent Linear Equations in n Unknowns, Computing, (1968), in press.

19. On Minimax Solutions of Linear Equations, submitted to Computer J., (1968).

20. A Least Squares Iterative Method for Singular Equations, Computer J., 12 (1969), pp. 388-392.

21. The Gaussian Elimination and Sparse Systems, "Sparse Matrix Proceedings", R. A. Willoughby Ed., IBM, Yorktown Heights (1969), pp. 35-42.

22. On the Use of Generalized Inverses in Function Minimization, submitted to Computing, 4 (1969), in press.

23. On the Transformation of Symmetric Sparse Matrices to the Triple Diagonal Form, International J. of Computer Mathematics, 2(1969), in press.

24. On the U-V Generalized Inverse of a Matrix, submitted to Lin. Alg. and Appl., (1969).

25. Computations with Sparse Matrices, SIAM Rev. 12(1970), forthcoming.

26. Sorting and Ordering Sparse Linear Systems, Proceedings of the Conference on Large Linear Systems, Oxford University, 1970, to appear.

27. On the Reduction of a Sparse Matrix to Hessenberg Form, Int. J. of Comp. Maths., 2(1970), to appear.

28. On Improving the Conditioning of the Coefficient Matrix of a System of Equations, (with V. N. Joshi), to be submitted.

29. Application of Boolean Methods for the Inversion of Sparse Matrices (with K. Y. Cheng), BIT(1970), submitted.

30. On Two Direct Methods for Computing Generalized Inverses, SIAM Rev. (1970), submitted.

REPORTS

1. A Direct Method for Generalized Matrix Inversion, Ibid., Report No. 70, (1966).

2. Solution of a System of Simultaneous Linear Equations with a Sparse Coefficient Matrix by Elimination Methods, Ibid., Report No. 85, (1967).

3. On the Chebyshev Solution of Inconsistent Linear Equations, Ibid., Report No. 106, (1968).

4. Some Comments on the Solution of Linear Equations, (with B. Ramnath), Ibid., Report No. 117, (1968).

5. The Gaussian Elimination and Sparse Systems, Ibid., Report No. 118, (1968).

6. Minimax Solution of n + 1 Inconsistent Linear Equations in n Unknowns, Ibid Report No. 121, (1968).

7. Applications of Generalized Inverses in the Solution of Linear Equations and Function Minimization, Ibid., Report No. 127, (1969).

8. On the Davidon-Fletcher-Powell Method for Function Minimization, Ibid., Report No. 140 (1969).

9. Sorting and Ordering Sparse Linear Systems, Report No. 151, (1970).

Abstracts in Notices of Amer. Math. Soc.,

1. Methods of Projection for the Solution of Sparse Linear System of Equations, Notices of AMS, Feb. 1968.

2. On the Chebyshev Solution of Inconsistent Linear Equations, Ibid., Aug. 1968.

. Presented papers and Lectures:

(a) Invited papers

1. Solution of Sparse Linear System of Equations, Numerical Analysis Workshop Meeting, NASA, Washington, D. C., January, 1968, NASA SP-170, p. 14 (abstract).
2. Solution of a System of Simultaneous Linear Equations with a Sparse Coefficient Matrix by Elimination Methods, "Operations Research Around the World Meetings," Madrid, Spain, July 28 - August 2, 1967.

3. The Elimination and the Orthogonalization Methods for the Inversion of Sparse Matrices, "Operations Research Around the World Meetings," New Delhi, India, August 7 -10, 1967.

4. A Method for Computing the Generalized Inverse of a Matrix,"Operations Research Around the World Meetings," Tokyo-Kyoto, Japan, August 14 - 18, 1967.

5. The Gaussian Elimination and Sparse Systems, "Symposium on Sparse Matrices and Applications" Yorktown Heights, N. Y., Sept. 9 - 10, 1968.

6. Applications of Graphy Theory to Sparse Matrices, Conference on Large set of Linear Equations, Oxford University, Oxford, England. April 5-9, 1970.

(b) Contributed papers

1. Graph Theoretic Interpretation of the Techniques for Minimizing the Densities of the Product Form of Inverses of Sparse Matrices, SIAM National Meeting, University of Iowa, Iowa City, Iowa, May, 1966, SIAM Rev., Vol. 8, No. 4, (1966) p. 579 (abstract).

2. On Computing Generalized Inverses, European Meeting on Statistics, Econometrics and Management Science, Amsterdam, Netherlands, Sept. 2 - 7, 1968.

3. On Chebyshev Solution of Inconsistent Linear Equations, Amer. Math. Soc. Meeting, Madison, Wisconsin, Aug. 27 - 30, 1968.

4. Reduction of a Sparse Matrix to Hessenberg Form, SIAM National Meeting, Denver, Colo., June 29-July 1, 1970.

(c) Lectures

1. "Generalized Inverses and Solution of Linear Equations". Two seminars for the faculty and students of Allahabad University, India. August, 1967.